Ignition Delay Times and Structure of Detonation Waves in $CH_4/O_2/N_2$ and $H_2/O_2/N_2$ Mixtures

FINAL REPORT

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Contents

1 Statement of the Problem Studied

In the research simplified chemical-kinetic mechanisms and reduced chemical-kinetic mechanisms were developed for describing 1) structures of the dark zone formed over the burning surface of solid propellants, 2) structures of premixed and nonpremixed flames burning various hydrocarbon fuels. Experimental, numerical and analytical studies were conducted. The results of the studies are described in the journal articles 1, 2, 3, 4, 5, and 6 listed in section 3.1, and in the technical reports 1, 2, and 3 listed in section 3.2. The journal articles 7, and 8 describe results of studies of the influence of bromotrifluromethane (CF_3Br), a commonly used fire suppressant, on the structures and critical conditions of extinction of nonpremixed methane flames and nonpremixed hydrogen flames. Simplified chemical kinetic mechanisms were developed for describing ignition delay times in combustible mixtures used in the Ram Accelerator. Summaries of the results of the research are described in section 2.

2 Summary of the Most Important Results

The summaries of the important results described in the journal articles listed in section 3 are given below.

2.1 Simplified Chemical-Kinetic Mechanisms for Characterizing the Structure of the Dark Zones of Double Base and Nitramine Propellants

This research is described in journal article 1 listed in section 3.1. The research was performed in collaboration with Dr. N. Ilincic in the Department of Applied Mechanics and Engineering Sciences (AMES) at the University of California at San Diego (UCSD), and with Dr. W. R. Anderson and Dr. N. E. Meagher at the U. S. Army Research Laboratory, Aberdeen Proving Ground, Maryland. Dr. N. Ilincic was a post-doctoral research staff in the Department of AMES at UCSD.

Simplified chemical-kinetic mechanisms were employed to calculate the structure of the dark zone formed over the burning surface of double base and nitramine propellants. It is believed that ignition delays in large caliber gun ballistic cycles are related to the chemistry taking place in the dark zone. Skeletal chemical-kinetic mechanisms comprising 22 elementary reactions among 15 species and 23 elementary reactions among 17 species were used to calculate the structure of the dark zone of double base and nitramine propellants, respectively. These skeletal chemical-kinetic mechanisms were previously extracted from a detailed chemical kinetic mechanism incorporating 190 elementary reactions involving 41 species. Ignition delay times were calculated using these mechanisms in homogeneous mixtures in which the initial concentrations of various reactants are similar to those found at the beginning of

the dark zones of double base and nitramine propellants. These calculations were performed for various initial pressures and temperatures. The ignition delay times calculated using the skeletal chemical-kinetic mechanisms were found to agree reasonably well with those calculated using the detailed chemical-kinetic mechanism. Reduced chemical-kinetic mechanisms were derived from the skeletal mechanisms by introducing steady-state approximations for a number of species. For double base propellants, a reduced mechanism of three global reactions was obtained. Reduced mechanisms utilizing six and four global reactions were deduced for nitramine propellants. The ignition delay times and structures of the dark zones calculated using the reduced three-step mechanism for double base propellants and six-step mechanism for nitramine propellants were in agreement with calculations made using the skeletal mechanisms. The ignition delay times calculated using the four-step reduced mechanism for nitramine propellants were found to be significantly smaller than those calculated using the skeletal mechanism. The reduced chemical-kinetic mechanisms are expected to be useful in interior ballistics calculations.

2.2 Numerical and Asymptotic Studies of the Structure of Stoichiometric and Lean Premixed Heptane Flames

This research is described in journal article 2 listed in section 3.1. The research was performed in collaboration with Professor N. Peters and Dr. M. Bollig at the Institut für Technische Mechanik, RWTH Aachen, Germany. Dr. M. Bollig was a graduate student at RWTH Aachen.

Numerical calculations and rate-ratio asymptotic analysis were performed to obtain the structure and burning velocities of premixed heptane flames. The numerical calculations were performed using a detailed chemical-kinetic mechanism comprising 257 elementary reactions, a skeletal chemical-kinetic mechanism comprising 34 elementary reactions and a reduced chemical-kinetic mechanism made up of six overall steps. The reduced chemical-kinetic mechanism was deduced from the skeletal mechanism. The rates of the overall reactions in the reduced mechanism were related to the rates of elementary reactions appearing in the skeletal chemical-kinetic mechanism. The values of burning velocities calculated numerically using the reduced chemical-kinetic mechanism were found to agree well with those calculated using the skeletal chemical-kinetic mechanism and the detailed chemical-kinetic mechanism.

The asymptotic structure of premixed heptane flames was analyzed using the reduced chemical-kinetic mechanism. The flame structure was presumed to consist of three zones— a pre-heat zone of thickness of order unity, a thin reaction zone, and a post-flame zone. In the pre-heat zone the rates of chemical reactions were presumed to be negligibly small. In the post-flame zone the products were presumed to be in chemical equilibrium and the temperature was presumed to be equal to the adiabatic flame temperature. In the reaction

5

zone the chemical reactions were presumed to take place in three layers—an inner layer, a C_2H_4-CH_2O consumption layer, and a H_2-CO oxidation layer. Within the inner layer there was a fuel-consumption layer of thickness of order δ where the fuel n-heptane was consumed and the intermediate hydrocarbon species C_2H_4 and CH_2O were formed. These intermediate hydrocarbon species were consumed in the C_2H_4-CH_2O consumption layer of thickness of order μ and CO and H_2 were formed. Most of the final products CO_2 and H_2O were formed in the H_2-CO oxidation layer which has a thickness of order ν. In the H_2-CO oxidation layer, H_2 was presumed to be in steady-state everywhere except in a thin sub-layer of thickness of order ϵ which was located within the H_2-CO oxidation layer. It was presumed that $\delta \ll \mu \ll \epsilon \ll \nu \ll 1$. The burning velocities calculated using the results of the asymptotic analysis were found to agree reasonably well with those calculated numerically using the skeletal chemical-kinetic mechanism and the detailed chemical-kinetic mechanism.

2.3 Structure and Extinction of Nonpremixed n-Heptane Flames

This research is described in journal article 3 listed in section 3.1. The research was performed in collaboration with Mr. R. Seiser, Mr. L. Truett, and Dr. D. Trees. Mr. R. Seiser and Mr. L. Truett are graduate students in the Department of AMES at UCSD and Dr. D. Trees was a postdoctoral research staff in the Department of AMES at UCSD.

An experimental and numerical study was performed to elucidate the structure and mechanisms of extinction of non-premixed n-heptane flames. Experiments were conducted on flames stabilized between two counterflowing streams. The fuel stream was a mixture of prevaporized n-heptane and nitrogen, and the oxidizer stream was a mixture of air and nitrogen. Concentration profiles of C_7H_{16}, O_2, N_2, CO_2, CO, H_2, CH_4, C_2H_2, C_2H_4, C_2H_6, C_3H_4, C_3H_6, C_3H_8, C_4-hydrocarbons, C_5-hydrocarbons, and C_6-hydrocarbons were measured. The measurements were made by removing gas samples from the flame using a quartz microprobe and analyzing the samples using gas chromatographs. The identity of the species was established using a mass selective detector. Temperature profiles were measured using a thermocouple. In addition, critical conditions of extinction were measured, giving the mass fraction of reactants as a function of the strain rate. Numerical calculations were performed using detailed chemistry to determine the flame structure and critical conditions of extinction at conditions identical to those used in the experiments. Calculated and measured flame structures were found to agree reasonably well, however, a small shift was observed between the calculated and measured temperature and concentration profiles. In general, the measured profiles were broader than the calculated profiles. At given values of the mass fraction of oxygen in the oxidizer stream, the calculated strain rates at extinction were noticeably higher than those measured. Experiments were also performed on non-premixed flames stabilized in the counterflowing configuration over a liquid pool of n-heptane. Critical conditions of extinction were measured.

Numerical calculations were performed at conditions used in these experiments and critical conditions of extinction were obtained. At given values of the mass fraction of oxygen in the oxidizer stream, the calculated strain rates at extinction were noticeably higher than those measured. The differences between the calculated and measured strain rates at extinction for the liquid pool flame were higher than for n-heptane-vapor flames.

2.4 Asymptotic Analyses of the Structure of Moderately Rich Methane-Air Flames

This research is described in journal article 4 listed in section 3.1. The research was performed in collaboration with Professor N. Peters and Dr. H. Pitsch at the Institut für Technische Mechanik, RWTH Aachen, Germany, and in collaboration with Dr. X. S. Bai at the Department of Heat and Power Engineering, Lund Institute of Technology, Sweden. Dr. H. Pitsch was a graduate student at RWTH Aachen.

The asymptotic structure of laminar, moderately rich, premixed methane flames was analyzed using a reduced chemical-kinetic mechanism comprising four global reactions. The reduced mechanism was different from those employed in asymptotic analyses of stoichiometric and lean flames, because a steady-state approximation was not introduced for CH_3. The aim of the analysis was to develop an asymptotic model for rich flames, that can predict the rapid decrease of the burning velocity with increasing equivalence ratio, ϕ. In the analysis, the flame structure was presumed to consist of three zones—a preheat zone with a normalized thickness of the order of unity, a thin reaction zone, and a post-flame zone. The preheat zone was presumed to be chemically inert, and in the post-flame zone the products were in chemical equilibrium and the temperature was equal to the adiabatic flame temperature, T_b. In the reaction zone the chemical reactions were presumed to take place in two layers: the inner layer and the oxidation layer. The rate constants of these reactions were evaluated at T^0, which is the characteristic temperature at the inner layer. In the inner layer the dominant reactions taking place were those between the fuel and radicals, and between CH_3 and the radicals. An important difference between the structure of the inner layer of rich flames and that of lean flames is the enhanced influence of the chain-breaking reaction, $CH_3 + H + (M) \rightarrow CH_4 + (M)$, in rich flames. Here M represents any third body. This reaction decreases the concentration of H radicals which in turn decreases the values of the burning velocity. In the oxidation layer of rich flames, the reactive-diffusive balance of O_2 was considered. This differs from the structure of the oxidation layer of lean flames where the reactive-diffusive balance of H_2 and CO was of primary interest.

The burning velocities calculated using the results of the asymptotic analysis were found to agree reasonably well with the burning velocities calculated numerically using chemical-kinetic

mechanisms made up of elementary reactions. The values of the characteristic temperature at the inner layer T^0 were found to increase with increasing values of the equivalence ratio and to approach T_b at $\phi = 1.36$. When T^0 is very close to T_b, the asymptotic analysis is not longer valid and an alternative asymptotic analysis must be developed for even larger equivalence ratios.

2.5 Multistep Asymptotic Analyses of Flame Structures

This research is described in journal article 5 listed in section 3.1. Aspects pertaining to rate-ratio asymptotic analyses of the structure of laminar unstretched premixed flames and non-premixed flames were described. The rate-ratio asymptotic analyses employ reduced chemical-kinetic mechanisms derived from detailed mechanisms. The rates of the global steps of the reduced chemical-kinetic mechanisms were related to the rates of elementary reactions.

The outer structure of premixed flames is presumed to comprise an inert preheat zone of thickness of the order of unity, a thin reaction zone where all chemical reactions take place, and a post flame zone where the products are in equilibrium. For methane, n-heptane, and methanol flames the reaction between the radicals and the fuel is chain-breaking. For *iso*-octane flames, the intermediate species *iso*-butene rather than the fuel depletes the radicals. This property was used to match the structure of the reaction zone with the structure of the chemically inert preheat zone. To obtain the burning velocity, it is necessary to analyze the structure of at least two reactive layers within the reaction zone—the inner layer and the oxidation layer. Qualitative features of the analyses of these layers in premixed methane flames are discussed. The characteristic temperature at the inner layer T^0 is found to play a central role in asymptotic analyses. It is calculated by comparing the rates of chain-breaking and chain-branching reactions and found to depend mainly on pressure. The burning velocity is found to be proportional to the difference between the adiabatic flame temperature and T^0. Therefore flame propagation cannot take place if the adiabatic flame temperature is lower than T^0. This shows that rate-ratio asymptotic analyses can provide a fundamental explanation for the existence of flammability limits. Characteristics of the analyses of the structure of hydrogen and wet carbon monoxide flames are also addressed. Rate-ratio asymptotic analyses of the structure of these flames are fundamentally different from those of hydrocarbon flames, because the reactions between these fuels and radicals are not chain-breaking.

Rate-ratio asymptotic analyses of nonpremixed flames are also described. The discussion is mainly focused on methane flames. The parameters that appear in the expression for the scalar dissipation rate at extinction are found to be similar to those for the burning velocity of premixed flames.

8

2.6 Rate-Ratio Asymptotic Analyses of Nonpremixed Methane Flames

This research is described in journal article 6 listed in section 3.1. The research was performed in collaboration with Dr. X. S. Bai at the Department of Heat and Power Engineering, Lund Institute of Technology, Sweden.

The asymptotic structure of laminar, nonpremixed methane flames was analyzed using a reduced four-step chemical-kinetic mechanism. Chemical reactions were presumed to take place in two layers: the inner layer and the oxidation layer. In the inner layer the fuel reacts with radicals and the main compounds formed were the intermediate species CO and H_2. These intermediate species were oxidized in the oxidation layer. The structure of the oxidation layer was described by two second order differential equations: one for CO and the other for H_2. Two limiting cases were considered. In one limit the global step $CO + H_2O \rightleftharpoons CO_2 + H_2$ was presumed to maintain partial equilibrium everywhere in the oxidation layer except in a thin layer adjacent to the inner layer. In the other limit steady-state approximation was introduced for H_2 everywhere in the oxidation layer except in a thin layer adjacent to the inner layer. The structure of the inner layer was described by two second order differential equations: one for the fuel and the other for the H-radicals. This is a significant improvement over previous models where either steady-state approximation was introduced for the H-radicals in the inner layer or the reaction between the fuel and radicals is presumed to be very fast. The chain-breaking elementary reaction $CH_3 + H + M \rightarrow CH_4 + M$ was found to have a significant influence on the structure of the inner layer and on the scalar dissipation rates at extinction. The influence of this reaction was either neglected in previous models or was included as a perturbation to the principal elementary reactions taking place to the leading order in the inner layer. Using the results of the asymptotic analysis the scalar dissipation rates at extinction were calculated at pressure of 1 bar. They were found to agree well with those calculated numerically using a chemical-kinetic mechanism made up of elementary reactions.

2.7 Rate-Ratio Asymptotic Analysis of Inhibition of Nonpremixed Methane-Air Flames by CF_3Br

This research is described in journal article 7 listed in section 3.1. The research was performed in collaboration with Dr. A. Grudno. Dr. A. Grudno was a visiting scholar from RWTH Aachen, Germany.

Rate-ratio asymptotic analysis was performed using a reduced four-step chemical-kinetic mechanism to elucidate the influence of CF_3Br on the structure of nonpremixed methane-air flames. The inhibitor CF_3Br was added to the oxidizing stream of the nonpremixed flame. The primary focus of the analysis was to obtain the critical conditions of extinction. The

asymptotic flame structure was constructed using the results of numerical calculations performed using a detailed chemical-kinetic mechanism made up of elementary reactions. The strain rate and the scalar dissipation rate represent the characteristic residence times in the reaction zone. For very small values of the strain rate and the scalar dissipation rate, the fuel CH_4 and the inhibitor CF_3Br were presumed to be consumed in different regions of the flame. The nondimensional distance between these regions was of the order of unity. At conditions close to extinction these regions merge and this merged reaction zone was analyzed.

In the merged reaction zone chemical reactions were presumed to take place in three layers which were called the fuel-consumption layer, the oxidation layer and the CF_3Br-consumption layer. The fuel was consumed in the fuel-consumption layer and the inhibitor in the CF_3Br-consumption layer. The elementary reaction $H + Br_2 \rightarrow HBr + Br$ was found to play a central role in the inhibition of the chemical reactions taking place in the flame. This reaction increases the rates by which radicals recombine in the oxidation layer. The results of the asymptotic analysis show that at fixed values of the scalar dissipation rate, with increasing concentrations of CF_3Br in the oxidizing stream the maximum temperature in the reaction zone increases, and the amount of oxygen leaking through the reaction zone increases. Also the scalar dissipation rates at extinction decrease with increasing concentrations of CF_3Br in the oxidizing stream. The qualitative aspects of the changes in the values of the scalar dissipation rate at extinction with increasing concentrations of CF_3Br agree well with numerical results obtained using a detailed chemical-kinetic mechanism and with experimental data.

2.8 Inhibition of Nonpremixed Hydrogen Flames by CF_3Br

This research is described in journal article 8 listed in section 3.1. The research was performed in collaboration with Mr. L. Truett, Mr. H. Thermann and Dr.. D. Trees in the Department of AMES at UCSD, and with Professor P. Marshall, Mr. J. Yuan, and Mr. L. Wells in the Department of Chemistry at University of North Texas, Denton, Texas. Mr. L. Truett is a graduate student in Department of AMES at UCSD and Dr. D. Trees was a postdoctoral research staff in the Department of AMES at UCSD. Mr. J. Yuan and Mr. L. Wells are graduate students in the Department of Chemistry at University of North Texas, Denton, Texas.

Experimental and numerical studies were performed to elucidate the fundamental chemical mechanisms by which CF_3Br inhibits nonpremixed hydrogen flames. These studies were motivated by previous work, which shows that CF_3Br and its decomposition products inhibit hydrocarbon flames primarily by reacting directly with the radicals and by depleting radicals in the region where hydrogen and carbon monoxide are oxidized to form water and carbon dioxide. The elementary reaction $CF_3Br + H = CF_3 + HBr$ plays a prominent role in flame inhibition, but there are considerable uncertainties in the value of the rate parameters for this

reaction. In view of these uncertainties, the rate of this reaction was measured directly by employing the flash-photolysis resonance fluorescence (FP-RF) technique and was compared with that predicted using transition state theory based on *ab initio* calculations. Predicted and measured rate parameters were found to agree well, but were found to differ significantly from those used in previous studies. The improved rate parameters were tested by conducting numerical computations and experiments on flames stabilized between two counterflowing streams. The fuel stream was a mixture of hydrogen and nitrogen and the oxidizing stream consisted of air and CF_3Br. The strain rate at extinction was measured and given as a function of the concentration of CF_3Br in the oxidizing stream. Numerical calculations were performed at conditions identical to those used in the experiments using detailed chemistry. Two different chemical-kinetic mechanisms were used. The chemical-kinetic mechanism describing the oxidation of the fuel was the same in both mechanisms, but the inhibition chemistries were different. One of the mechanisms has not been tested before on nonpremixed flames. One mechanism was found to generally overpredict and the other to underpredict the inhibiting effect of CF_3Br. The degree of overprediction and underprediction was evaluated using asymptotic theory.

2.9 Simplified Mechanisms for Calculating Ignition Delay Times in Reactive Mixtures Employed in the RAM Accelerator

Simplified and reduced chemical-kinetic mechanisms were obtained for calculating ignition delay times in reactive mixtures employed in the RAM accelerator. The skeletal mechanism was made up of 90 elementary reactions among the 22 reactive species. This skeletal mechanism was deduced from a detailed chemical-kinetic mechanism made up of 552 elementary reactions among 44 reactive species. Reduced chemical-kinetic mechanisms made up of fourteen overall steps and eleven overall steps were deduced from the skeletal mechanism. Calculations were performed assuming constant volume conditions for reactive mixtures $3CH_4 + 2O_2 + 10N_2$ for various values of the pressure and initial temperature of the reactants. The ignition delay times calculated using the skeletal and reduced fourteen-step mechanism were found to agree well with those calculated using the detailed mechanism.

3 List of all Publications and Technical Reports

3.1 Journal Articles

1. Ilincic, N., Anderson, W. R., Seshadri, K., and Meagher, N. E., "Simplified Chemical-Kinetic Mechanisms for Characterizing the Structure of the Dark Zones of Double Base and Nitramine Propellants," *Twenty-Sixth Symposium (International) on Combustion*, The Combustion Institute, 1996, pp 1997–2006.

2. Seshadri, K., Bollig, M., and Peters, N., "Numerical and Asymptotic Studies of the Structure of Stoichiometric and Lean Premixed Heptane Flames, " *Combustion and Flame,* **108**, Number 4, 1997, pp 518–536.

3. Seiser, R., Truett, L., Trees, D., and Seshadri, K., "Structure and Extinction of Nonpremixed *n*-Heptane Flames," *Twenty-Seventh Symposium (International) on Combustion,* The Combustion Institute, 1998, pp 649–657.

4. Seshadri, K., Bai, X. S., Pitsch, H., and Peters, N., "Asymptotic Analyses of the Structure of Moderately Rich Methane-Air Flames," *Combustion and Flame,* **113**, 1998, pp 589–602.

5. Seshadri, K., "Multistep Asymptotic Analyses of Flame Structures," Invited Topical Review, *Twenty-Sixth Symposium (International) on Combustion,* The Combustion Institute, 1996, pp 831–846.

6. Bai, X. S., and Seshadri, K., "Rate-Ratio Asymptotic Analysis of Nonpremixed Methane Flames," *Combustion Theory and Modelling,* **3**, 1999, pp 51–75.

7. Grudno, A., and Seshadri, K., "Rate-Ratio Asymptotic Analysis of Inhibition of Nonpremixed Methane-Air Flames by CF_3Br," *Combustion and Flame,* **112**, 1998, pp 418–437

8. Truett, L., Thermann, H., Trees, D., Seshadri, K., Yuan, J., Wells, L., and Marshall, P., "Inhibition of Nonpremixed Hydrogen Flames by CF_3Br," *Twenty-Seventh Symposium (International) on Combustion,* The Combustion Institute, 1998, pp 2741–2748.

3.2 Papers Published in Proceedings of Technical Meetings

1. Anderson, W. R., Ilincic, N., Meager, N. E., Seshadri, K., and Vanderhoff, J. A., "Detailed and Reduced Chemical Mechanisms for the Dark Zones of Double and Nitramine Propellants in the Intermediate Temperature Regime," Proceedings of the 32nd JANNAF Combustion Meeting, 1995.

2. Anderson, W. R., Ilincic, N., Meagher, N. E., Seshadri, K., and Vanderhoff, J. A., "Chemical Mechanisms for the Dark Zones of Double Base and Nitramine Gun Propellants for Interior Ballistic Modeling," 20th Army Science Conference, Paper # E-P6, Norfolk, Virginia, June 1996.

3. Ilincic, N., Anderson, W. R., and Seshadri, K., "Development of a Reduced Mechanism for the Double Base Propellant Dark Zone," AIAA paper # 96-0649, 34th Aerospace Sciences Meeting and Exhibit, January 15–18, 1996, Reno, Nevada.

4. Seiser, R., Trees, D., Pitsch, H., and Seshadri, K., "Extinction and Ignition of Hydro-carbon Fuels," Proceedings of the Joint Meeting of the United States Sections of the Combustion Institute, The George Washington University, Washington, DC, March 15, 16, and 17, 1999, pg 236–239.

5. Trees, D., Seshadri, K., Anderson, W. R. and Meagher, N. E., "Ignition Delay Times of Dark Zone Mixtures of Double Base and Nitramine Propellants," Proceedings of the Joint Meeting of the United States Sections of the Combustion Institute, The George Washington University, Washington, DC, March 15, 16, and 17, 1999, pg 733–736.

4   Participating Scientific Personnel

The participating scientific personnel were 1) Professor K. Seshadri, 2) Dr. N. Ilincic, 3) Dr. D. Trees, and 4) Mr. R. Seiser. Drs. Ilincic and D. Trees were postdoctoral research staff. Mr. R. Seiser is a graduate student.

5   Report of Inventions

None.

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13. ABSTRACT *(Maximum 200 words)*

Simplified chemical-kinetic mechanisms and reduced chemical-kinetic mechanisms were developed for describing structure of the dark zone formed over the burning surface of double base and nitramine propellants. It is believed that ignition delays in large caliber gun ballistic cycles are related to the chemistry taking place in the dark zone. Ignition delay times calculated using the simplified mechanisms were found to agree well with those calculated using detailed chemical-kinetic mechanisms. The simplified mechanisms are expected to be useful in interior ballistics calculations. Reduced chemical-kinetic mechanisms were developed to calculate the structures of premixed and nonpremixed flames burning various hydrocarbon fuels. Asymptotic analyses were performed using the reduced mechanisms. Burning velocities of premixed flames and critical conditions of extinction of nonpremixed flames were calculated using results of the asymptotic analyses. Simplified chemical-kinetic mechanisms were developed for calculating ignition delay times in combustible mixtures used in the Ram Accelerator. The results of all these studies are described in eight journal articles and five technical reports published in proceedings of technical meetings.

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